

# Optoelectronic properties of the new quaternary chalcogenides $\text{Zn}_2\text{CuInTe}_4$ & $\text{Cd}_2\text{CuInTe}_4$ : ab-initio study.

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**Abstract:** In order to exploit the fundamental properties of the new tellurides quaternary diamond-like structure  $\text{Zn}_2\text{CuInTe}_4$  and  $\text{Cd}_2\text{CuInTe}_4$ , first principles investigation in the framework of the Full-Potential LAPW scheme have been carried out for that purpose. We used the Wu and Cohen generalized gradient approximation (GGA-WC) to calculate the optimized structure that corresponds to the global minima of the energy. Enthalpy of formation shows that the most stable structures are the relaxed ones. The EV-GGA and the TB-mBJ approximations were also used for electronic and optical properties. The equilibrium electronic parameters found are in good agreement with the previous results. The real and the imaginary parts of the dielectric function, the refractive index, the extinction coefficient, the absorption coefficient, the loss function and the reflectivity are reviewed in the large spectral range of photon energy. The present study demonstrates a variety of novel electronic and optical properties, which make these compounds highly promising for optoelectronic materials.

**Keywords :** DFT, Quaternary tellurides, Enthalpy of formation, band gap, Absorption coefficient